B.TECH/CHE/7TH SEM(L)/CHE 704A/2021

NUMERICAL METHODS IN CHEMICAL ENGINEERING
(CHE 704A)

Time Allotted : 3 hrs **Full Marks : 70**

The questions are of equal value.
The figures in the margin indicate full marks
Candidates are required to give answer in their own words as far as practicable.
All symbols are of usual significance.

Group – A
(Multiple Choice Type Questions)

1. Choose the correct alternative for the following (any ten): **10 × 1 = 10**

(i) If S_T be the total error, S_R be the residual error then the regression coefficient value will be give as

(a) $r^2 = \frac{S_R}{S_T}$ (b) $r^2 = \frac{S_T - S_R}{S_T}$

(c) $r^2 = \sqrt{\frac{S_T - S_R}{S_T}}$ (d) None of these.

(ii) When the stiffness depends on some linear assumption as $y' = \lambda t$ The stability criterion for Euler's method can be given as

(a) $\lambda < 0$ (b) $\lambda > 0$ and $h < \frac{2}{\lambda}$

(c) $\lambda > 0$ and $|1-\lambda h| \leq 1$ (d) All of these.

(iii) If one does not know the order of the polynomial, for interpolation at any point
(a) Lagrangian interpolation can be used
(b) Newton's divided difference scheme can be used
(c) Both (a) and (b) can be used
(d) None of these can be used.

(iv) Shooting method can be used for ordinary differential equations, which are
(a) Initial value problem
(b) Boundary value problem
(c) Both (a) and (b)

(d) In case of Boundary value problem, when the initial condition is defined for the extreme boundary

(v) To approximate a first order differential term in $O(h^2)$ the expansion can be given as

(a) $\frac{dy_i}{dx} = \frac{1}{2h}(3y_i - 4y_{i-1} + y_{i-2}) + O(h^2)$

(b) $\frac{dy_i}{dx} = \frac{1}{2h}(y_i - 2y_{i-1} + y_{i-2}) + O(h^2)$

(c) Both (a) and (b)

(d) None of these

(vi) Transient temperature response in a copper wire held at two different temperatures at both ends results in

(a) An elliptic PDE (b) A parabolic PDE

(c) An elliptic and parabolic PDE (d) None of the above.

(vii) Truncation errors can be predicted through

(a) Calculating round-off errors (b) Taylor series approximation

(c) Analysis of the Fibonacci series (d) None of the above.

(viii) The underlying principle in Muller's method is

(a) Estimating a root by projecting a straight line to the x axis

(b) Estimating root by projecting a parabola through 3 points

(c) Estimating a root by fitting a polynomial through 5 points

(d) None of the above.

(xi) Successive overrelaxation factor is used in

(a) Iterative methods for solving linear systems

(b) Is used to obtain rapid convergence of Newton Raphson method

(c) Is used in conjunction with Gaus Siedel for faster convergence

(d) Both (a) and (c).

(x) A Tridiagonal matrix is formed in the solution of

(a) A parabolic PDE in one dimension in space

(b) An elliptic PDE in two dimension in space

(c) Never encountered in PDEs

(d) None of the above.

(xi) The restrictions of the time-explicit scheme is that

(a) $\Delta t \le \frac{\Delta x^2}{4\alpha}$ (b) $\Delta t \le \frac{\Delta x^2}{2\alpha}$ (c) $\Delta t^2 \le \frac{\Delta x^2}{4\alpha}$ (d) $\Delta t \le \left(\frac{\Delta x}{2\alpha}\right)^2$

(xii) Crank-Nicholson scheme uses
(a) A time implicit method of solving PDE
(b) A time explicit method of solving PDE
(c) The average of Second derivatives at two different times
(d) None of the above.

Group – B
(Short Answer Type Questions)

Answer any three of the following: **3 × 5 = 15**

2. With the following fermentation data develop the polynomial function using Newton's forward difference table

Time (h)	Penicillin concentration (units/mL)	Time (h)	Penicillin concentration (units/mL)
0	0	120	9430
20	106	140	10950
40	1600	160	10280
60	3000	180	9620
80	5810	200	9400
100	8600		

3. For a liquid level PI controller the characteristic equation is written as,

$$\frac{d^2h}{dt^2} - 3\frac{dh}{dt} - 10h = 0, \text{when } h(0) = 3 \text{ and } \frac{dh(0)}{dt} = 15$$

Find the rate of change of liquid level in the storage tank (having both inlet and outlet) after 1 min using fourth order Runge-Kutta method, when the data is recorded at 1 minute interval.

4. The volume V of liquid in a hollow horizontal cylinder of radius r and length L is related to the depth of the liquid h by

$$V = \left[r^2 \cos^{-1}\frac{r-h}{h} - (r-h)\sqrt{2rh-h^2} \right] L$$

Determine h using Newton Raphson method. given r = 2m, L = 5m, and V = 8.5m3 (Show one .

5. In between Simpson's 1/3rd rule and trapezoidal rule, which one provides maximum accuracy in integrating a function within a limit and why?

Group – C
(Long Answer Type Questions)

Answer any three of the following: **3 × 15 = 45**

6. A plug flow reactor is to be designed to produce product D from A according to the following reaction
A → D, where $r_D = 60C_A$ mole of D/L.s
In the operating condition of this reactor, the following undesired reaction took place:
A → U, where $r_U = \frac{0.003C_A}{1+10^5 C_A}$ mole of U / L.s
The undesired product U is a pollutant and it costs 10$/mole of U to dispose it, where as the desired product D has a value of 35$/mole of D. What should be the size of the reactor in order to obtain an effluent stream at its maximum value? Pure reactant A with volumetric flow rate of 15 L/s and molar flow rate of 0.1mol/s enters the reactor. Value of A is 5$/mole of A. Solve the system using 4th order Adams-Bashforth-Moulton predictor-corrector method. Show two time steps with 1 s interval.
Adams-Bashforth scheme:

$$y_{i+1} = y_i + h\sum_{k=0}^{n}\beta_k f_{i-k}$$

$$\beta_0 = \frac{55}{24}, \beta_1 = -\frac{59}{24}, \beta_2 = \frac{37}{24}, \beta_3 = -\frac{9}{24}$$

Adams-Moulton scheme:

$$y_{i+1} = y_i + h\sum_{k=0}^{n}\beta_k f_{i+1-k}$$

$$\beta_0 = \frac{9}{24}, \beta_1 = \frac{19}{24}, \beta_2 = -\frac{5}{24}, \beta_3 = \frac{1}{24}$$

15

7. Calculate the terminal velocity using Newton Raphson method of coals for particles with the following parameters ρp = 1800 kg/m3; Dp = 208 mm; at 25OC ρ=1000 kg/m3; μ=8.9x10-3 Pas; CD=24/Re for Re<0.1 and $u_t = \sqrt{\frac{4g(\rho_P - \rho)D_P}{3C_D\rho}}$. Show maximum three iterations.

15

8. (a) An ice cream company makes three ice-cream blends: LimeOrange, using 2 gallons of lime ice cream and 2 gallons of orange ice cream per gallon; LimeLemon, using 3 gallons of lime ice cream and 1 gallon of lemon ice cream per gallon; and OrangeLemon, using 3 gallons of orange ice cream and 1 gallon of lemon ice cream per gallon. Each day the company has 800 gallons of lime ice cream, 650 gallons of orange ice cream, and 350 gallons of lemon ice cream available. How many gallon of each blend should it make each day if it wants to use up all of the supplies?
(b) What is partial pivoting? Demonstrate with an example when you should be using it?

9 + 6 = 15

9. (a) Water solubility in jet fuel, WS, as a function of temperature, T, has been measured and the following experimental data reported.

T (oC)	-40	-20	0	20	40
WS	0.0012	0.002	0.0032	0.006	0.0118

Use Newton's interpolation to obtain values at 5^{o}C.
(b) If a lagrange polynomial were to be fitted to above data, evaluate the coefficients and state the order of polynomial used.

9 + 6 = 15

10. Write short notes on any *three* of the following **(3 x 5) = 15**
    a) Bisection Method
    b) Gauss Jordon Elimination
    c) Heun's method
    d) Tridiagonal matrix algorithm
    e) Round-off errors.

Department & Section	Submission Link
CHE	Class Code skahpps
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